Construction of the center-of-mass free space
for the SU(3) no-core shell model

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Abstract

We address the removal of states with center-of-mass excitation from the SU(3) no-core shell model [SU(3)-NCSM] space, *i.e.*, construction of the nonspurious subspace. A procedure is formulated based on solution of the null-space problem for the center-of-mass harmonic oscillator lowering operator $\tilde{B}_{\text{c.m.}}^{(01)}$, operating at the level of SU(3) irreducible representations. Isolation of the center-of-mass free subspace for the SU(3)-NCSM provides the foundation for exact removal of center-of-mass dynamics in the proposed $\text{Sp}(3, \mathbb{R})$ symplectic no-core shell model. We outline the construction process for the matrix representation of $\tilde{B}_{\text{c.m.}}^{(01)}$, present the algorithm for obtaining the nonspurious space, and examine the dimensions obtained for center-of-mass free SU(3) subspaces in representative light nuclei.

Keywords: SU(3) no-core shell model, spurious excitations, center-of-mass free space

1. Introduction

The ability to carry out no-core configuration interaction calculations of light nuclei, in the no-core shell model (NCSM) [1–3], has made a significant contribution to recent progress in the *ab initio* description of nuclei. However, the dimensionality of the nuclear model space becomes computationally prohibitive as the number of active nucleons and orbitals increases. Symmetry can play a significant role in addressing this problem, by assisting in the selection of the physically relevant portions of the model space. Elliott [4–6] explored the U(3) ⊃ SU(3) symmetry of the harmonic oscillator, which serves as an organizational scheme for quadrupole deformation and rotation in the nuclear shell model. The U(3) algebra of the oscillator is contained in a larger $\text{Sp}(3, \mathbb{R})$ algebra, which is found to have a close connection both to the dominant components of the nuclear Hamiltonian and to nuclear collective motion [7–9]. Following the discovery of evidence for SU(3) and $\text{Sp}(3, \mathbb{R})$ symmetry in the nuclear eigenstates obtained in conventional NCSM calculations for light nuclei [10, 11], the NCSM has been reformulated in terms of an SU(3)-based model space, in the SU(3) no-core shell model [SU(3)-NCSM] [12, 13]. This development provides the foundations for future realization of a symplectic no-core shell model (Sp-NCSM) [14], making full use of $\text{Sp}(3, \mathbb{R})$ symmetry.

In predicting physical properties of the nucleus, only the intrinsic dynamics of the nucleus is of interest, not the center-of-mass motion. In principle, the center-of-mass

motion may be eliminated from the problem by explicitly changing variables to relative coordinates. However, the nuclear many-body state must be antisymmetrized, and with increasing nucleon number this process rapidly becomes prohibitive in relative coordinates [3]. On the other hand, for a many-body basis constructed from antisymmetrized products of single-particle states, as in the NCSM, antisymmetrization is straightforward, but both center-of-mass (spurious) and intrinsic excitations are included in the model space [15, 16]. Consequently many of the nuclear eigenstates obtained by diagonalizing the Hamiltonian will carry center-of-mass excitation. Moreover, exact factorization of the many-body wave function into center-of-mass and intrinsic parts — *i.e.*, $\psi(\vec{r}_i; \vec{\sigma}_i) = \psi_{\text{c.m.}}(\vec{R})\psi_{\text{in}}(\vec{r}_{ij}; \vec{\sigma}_i)$, where $\psi_{\text{c.m.}}(\vec{R})$ depends on the center-of-mass coordinate, and $\psi_{\text{in}}(\vec{r}_{ij}; \vec{\sigma}_i)$ depends on relative coordinates $\vec{r}_{ij}$ and intrinsic spin degrees of freedom — is obtained only within certain specific truncations of the model space. In the context of the conventional NCSM, for which the basis is constructed from antisymmetrized products of oscillator wave functions, factorization is obtained if truncation is carried out according to the N_{max} scheme, that is, by the total number of oscillator quanta for the many-body state [3]. Within the SU(3)-NCSM, factorization is also retained in model spaces which have furthermore been truncated according to SU(3) and spin quantum numbers (see Section 3). Otherwise, factorization of intrinsic and center-of-mass wave functions is in general incomplete, in which case all eigenstates contain some spurious contribution, presenting challenges for the study of the intrinsic excitations (*e.g.*, Refs. [17–19]).

The usual approach to addressing the problem of spurious states consists of modifying the nuclear *Hamiltonian*, working within a model space which supports factorization, by adding a Lawson term [20] proportional the harmonic oscillator Hamiltonian $H_{\text{c.m.}}$ for the center-of-mass coordinate. After diagonalization, the spurious states remain in the spectrum but are shifted to an excitation energy above the low-lying intrinsic states of interest. However, the other possibility is to modify the *model space*, so as to explicitly remove the entire space of spurious states, before the Hamiltonian is diagonalized. This approach may be made feasible through the use of SU(3) symmetry [21–25]. After the spurious states are removed, the remaining center-of-mass free (CMF) states form a suitable model space for describing the intrinsic dynamics of the nucleus.

The CMF states are associated with the lowest eigenvalue of the center-of-mass Hamiltonian $H_{\text{c.m.}}$ and thus possess a harmonic oscillator $0s$ wave function in the center-of-mass degrees of freedom. They also therefore constitute the null space of the center-of-mass harmonic oscillator lowering operator $\tilde{B}_{\text{c.m.}}^{(01)}$. The approach developed here for isolating the CMF space is based on solution of the null-space problem for this operator, formulated at the level of subspaces of definite SU(3) symmetry and intrinsic spin.

A principal motivation is to enable exact separation of center-of-mass dynamics in extensions to the SU(3)-NCSM, in particular the Sp-NCSM. The many-body basis for the SU(3)-NCSM is the starting point for defining the basis for the Sp-NCSM [14]. Briefly, an $\text{Sp}(3,\mathbb{R})$ irreducible representation (irrep) is constructed from an extremal SU(3) state [14], *i.e.*, possessing the fewest oscillator quanta. Other states within the irrep are constructed by acting on this extremal state with an SU(3)-coupled product $[A^{(20)} \times A^{(20)} ... \times A^{(20)}]^{(\lambda\mu)}$, where $A^{(20)}$ is the translationally-invariant $\text{Sp}(3,\mathbb{R})$ raising operator. Each application of $A^{(20)}$ contributes two oscillator quanta to the system. Since the action of $A^{(20)}$ does not introduce center-of-mass excitation, an $\text{Sp}(3,\mathbb{R})$ irrep is free of center-of-mass excitation as long as it is built from an extremal SU(3) state

which is free of such excitation. The present results therefore provide the foundation for obtaining the CMF model space for the Sp-NCSM.

The construction of the SU(3)-NCSM basis, before removal of spurious contributions, is first outlined (Section 2). We then introduce an algorithm for identification of the CMF subspace within the SU(3)-NCSM model space, based on constructing the matrix representation of $\tilde{B}_{\mathrm{c.m.}}^{(01)}$ between SU(3)-coupled subspaces and solving for its null space (Section 3). Finally, we summarize the dimensions obtained for CMF SU(3) subspaces in representative light nuclei (Section 4). Preliminary results were reported in Ref. [26].

2. SU(3)-NCSM basis states

The many-body basis states for the SU(3)-NCSM have good $SU(3) \times SU(2)$ quantum numbers, where the SU(3) symmetry label $(\lambda\mu)$ characterizes the spatial degrees of free-dom, according to the Elliott classification, while the SU(2) label S describes the total intrinsic spin angular momentum. The creation operator for a nucleon in a given major oscillator shell η comprises an $SU(3) \times SU(2)$ tensor $a_{(\eta 0)1/2}^{\dagger}$, where the labels denote $(\lambda\mu)S = (\eta 0)\frac{1}{2}$ [27]. The operators $a_{(\eta 0)1/2}^{\dagger}$ are then used as the fundamental units in building up an $SU(3) \times SU(2)$-coupled nuclear state.

Specifically, each SU(3)-NCSM basis state is characterized by a definite distribution of nucleons over the major shells. First, all nucleons in the each major shell η are combined to form a configuration of the type $[a_{(\eta 0)1/2}^{\dagger} \times a_{(\eta 0)1/2}^{\dagger} \times \cdots]^{(\lambda_\eta \mu_\eta)S_\eta}$, with good $SU(3) \times SU(2)$ coupling [28], separately for the protons and neutrons. Then, such configurations for individual major shells are coupled successively to form a total proton state and total neutron state carrying good $SU(3) \times SU(2)$ quantum numbers. Finally, the proton state and neutron state are coupled, to give the SU(3)-NCSM basis state. Since the major shells have definite occupations, the state may be classified, as usual in the oscillator basis for the NCSM [3], by the number N_{ex} of harmonic oscillator excitations, taken relative to the minimal number of oscillator quanta possible for the given number of protons and neutrons.

The resulting SU(3)-NCSM basis state has the form, with all coupling labels shown explicitly,

$$\Big(|((((\gamma_{p,0} \times \gamma_{p,1})^{\rho_{p,0}\omega_{p,0}} \times \gamma_{p,2})^{\rho_{p,1}\omega_{p,1}} \times \gamma_{p,3})^{\rho_{p,2}\omega_{p,2}} ... \times \gamma_{p,\eta_{\max}})^{\rho_p \omega_p}\rangle$$

$$\times |((((\gamma_{n,0} \times \gamma_{n,1})^{\rho_{n,0}\omega_{n,0}} \times \gamma_{n,2})^{\rho_{n,1}\omega_{n,1}} \times \gamma_{n,3})^{\rho_{n,2}\omega_{n,2}} ... \times \gamma_{n,\eta_{\max}})^{\rho_n \omega_n}\rangle \Big)^{\rho\omega}. \quad (1)$$

Here the symbol $\gamma_{s,\eta}$ represents the labels $\gamma = [f_1, f_2, \ldots, f_N]\alpha(\lambda\mu)S$ needed to completely specify the coupling of nucleons of type s (*i.e.*, protons or neutrons) within major shell η [28]. Specifically, each major shell has associated with it a U(N) algebra $[N = (\eta + 1)(\eta + 2)]$ consisting of bilinears of creation and annihilation operators, for which the irreps are labeled by $[f_1, f_2, \ldots, f_N]$, where we consider only antisymmetric irreps, and $\sum_{i=1}^{N} f_i$ equals the occupation of the shell. Within a U(N) irrep, a multiplicity index α is required to distinguish $SU(3) \times SU(2)$ irreps with the same quantum numbers $(\lambda\mu)S$, yielding the labeling scheme

$$
\begin{array}{ccc}
\mathrm{U}(N) & \supset & \mathrm{SU}(3) \times \mathrm{SU}(2) \, . \\
[f_1, f_2, \ldots, f_N] & \alpha \quad (\lambda\mu) & S
\end{array}
\quad (2)
$$

The symbols $\omega_{s,\eta}$ in (1) then indicate the $SU(3) \times SU(2)$ coupling labels $[\omega \equiv (\lambda\mu)S]$ of successive shells, and $\rho_{s,\eta}$ denotes the multiplicity index for this coupling. Finally we have total couplings $\omega_p \equiv (\lambda_p\mu_p)S_p$ for the protons, $\omega_n \equiv (\lambda_n\mu_p)S_n$ for the neutrons, and $\omega \equiv (\lambda\mu)S$ for the entire basis state, with corresponding multiplicity indices ρ_p, ρ_n, and ρ, respectively.

The expression in (1) represents not just a single state but an entire set of states, with various values for the quantum numbers associated with the branching of $SU(3) \times SU(2)$ into angular momentum subalgebras: the orbital (spatial) angular momentum L, the inner multiplicity κ for this L within the $SU(3)$ irrep $(\lambda\mu)$, and the total angular momentum J, as well as its z-projection M. However, these states share the same "internal" microscopic structure, given by the same couplings of the particles at the level of $SU(3) \times SU(2)$. Therefore, they may be thought of as a single *reduced state* for certain purposes, in particular, evaluation of reduced matrix elements under the $SU(3) \times SU(2)$ Wigner-Eckart theorem and, as we shall see, identification of CMF linear combinations. The analogy is to angular momentum theory, where one may consider the states $|JM\rangle$, for different M, to be substates of a single state $\|J\rangle$, more formally, a tensorial set or $SU(2)$ irrep.

3. Construction of the CMF subspace

The separation of the many-body space into CMF and spurious parts simplifies in the context of an $SU(3) \times SU(2)$-coupled basis, since the process may be carried out independently within subspaces characterized by definite $SU(3) \times SU(2)$ quantum numbers. To start with, the center-of-mass Hamiltonian $H_{\mathrm{c.m.}}$ does not connect states involving different numbers N_{ex} of oscillator excitations, *i.e.*, $[H_{\mathrm{c.m.}}, \hat{N}_{\mathrm{ex}}] = 0$. It is due to this property that the usual $N_{\max}$ truncation scheme for the NCSM [3] permits an exact factorization of center-of-mass and intrinsic wave functions.[1] This property also implies that the separation of CMF states may be carried out separately within the space of states with each specific number of oscillator quanta, which we denote by $W_{N_{\mathrm{ex}}}$. Furthermore, $H_{\mathrm{c.m.}}$ commutes with the $SU(3)$ generators and may therefore be diagonalized within a subspace with good $SU(3)$ quantum numbers [22]. As an operator acting only on spatial degrees of freedom, $H_{\mathrm{c.m.}}$ also commutes with the total spin operators for protons and neutrons, as well as their combined spin operator. Thus, collecting these properties, the separation of CMF states may be carried out separately within subspaces of given N_{ex}, $(\lambda\mu)$, S_p, S_n, and S, which we denote by $W_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]$.

In considering how to extract CMF states, we note that these states are defined by their relation to the center-of-mass harmonic oscillator raising and lowering operators. The center-of-mass raising operator $B_{\mathrm{c.m.}}^\dagger$, which is an $L = 1$ operator, furthermore constitutes an $SU(3)$ (10) tensor, with components $B_{\mathrm{c.m.},L=1,M}^{\dagger(10)}$. This operator may be written in terms of single-particle harmonic-oscillator raising operators $b^{\dagger(10)}$ as [14, 27]

$$B_{\mathrm{c.m.}}^{\dagger(10)} = \frac{1}{\sqrt{A}} \sum_{i=1}^{A} b^{\dagger(10)}(i). \tag{3}$$

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[1]The $N_{\max}$ truncation is to many-body states with $0 \leq N_{\mathrm{ex}} \leq N_{\max}$. For NCSM calculations with parity-conserving interactions, the two parity subspaces, obtained for N_{ex} even or odd, respectively, may furthermore be considered separately.

The corresponding lowering operator $\tilde{B}_{\text{c.m.}}^{(01)}$ similarly has the form

$$\tilde{B}_{\text{c.m.}}^{(01)} = \frac{1}{\sqrt{A}} \sum_{i=1}^{A} \tilde{b}^{(01)}(i). \tag{4}$$

The center-of-mass harmonic oscillator Hamiltonian is built from these operators as

$$H_{\text{c.m.}} = \hbar\omega\Big(B_{\text{c.m.}}^{\dagger(10)} \cdot \tilde{B}_{\text{c.m.}}^{(01)} + \frac{3}{2}\Big), \tag{5}$$

where the dot indicates a spherical tensor scalar product. The CMF states are then defined by the property that they have no center-of-mass excitations, *i.e.*, they have zero eigenvalue for the center-of-mass number operator $N_{\text{c.m.}} = B_{\text{c.m.}}^{\dagger(10)} \cdot \tilde{B}_{\text{c.m.}}^{(01)}$. Equivalently, however, they are identified by the property that they are annihilated by the center-of-mass lowering operator $\tilde{B}_{\text{c.m.}}^{(01)}$.

Either of these criteria allow the problem of identifying CMF states to be formulated as a null-space problem. We seek the subspace $W_{N_{\text{ex}}}^{\text{CMF}}[(\lambda\mu)S_pS_nS]$ of $W_{N_{\text{ex}}}[(\lambda\mu)S_pS_nS]$ consisting of states $|\Psi^{\text{CMF}}\rangle$ such that $N_{\text{c.m.}}|\Psi^{\text{CMF}}\rangle = 0$ or, equivalently, $\tilde{B}_{\text{c.m.},L=1,M}^{(01)}|\Psi^{\text{CMF}}\rangle = 0$. In practice, this means first representing the operator as a matrix with respect to the SU(3)-NCSM basis and then solving for a complete set of null vectors of this matrix. The result yields new basis states, for $W_{N_{\text{ex}}}^{\text{CMF}}[(\lambda\mu)S_pS_nS]$, as linear combinations of the original basis states, for $W_{N_{\text{ex}}}[(\lambda\mu)S_pS_nS]$.

Although we could in principle search for the null space of either $N_{\text{c.m.}}$ or $\tilde{B}_{\text{c.m.}}^{(01)}$, there is a practical advantage to working with $\tilde{B}_{\text{c.m.}}^{(01)}$. While $N_{\text{c.m.}}$ is a two-body operator, $\tilde{B}_{\text{c.m.}}^{(01)}$ is simply a one-body operator. Consequently, evaluation of matrix elements is computationally less involved. Note that $N_{\text{c.m.}}$ acts within the space $W_{N_{\text{ex}}}$, *i.e.*, conserving the number of oscillator excitations, but $\tilde{B}_{\text{c.m.}}^{(01)}$ connects the space $W_{N_{\text{ex}}}$ to the next lower space $W_{N_{\text{ex}}-1}$, which is significantly smaller in dimension than $W_{N_{\text{ex}}}$. One might therefore expect the null space problem for $\tilde{B}_{\text{c.m.}}^{(01)}$ to be of lower dimensionality than that for $N_{\text{c.m.}}$, namely, involving a matrix of the same column dimension ($\sim \dim W_{N_{\text{ex}}}$) but lower row dimension ($\sim \dim W_{N_{\text{ex}}-1}$). However, this simple relation of dimensions is modified once SU(3) selection rules are considered (see below), and in practice the difference in dimensionality of the two problems is largely eliminated.

The problem of identifying CMF states is simplified by the realization that it may be formulated entirely at the level of reduced states. Recall that $H_{\text{c.m.}}$ commutes with the SU(3) generators, which connect states within an irrep. Consequently, an SU(3) $\times$ SU(2)-reduced state is CMF if and only if its substates, labeled by κLJ (and M), are all CMF. We need thus only find a basis of SU(3) $\times$ SU(2)-*reduced* states, for $W_{N_{\text{ex}}}^{\text{CMF}}[(\lambda\mu)S_pS_nS]$, independent of κLJM. We also need only consider the SU(3) $\times$ SU(2)-*reduced* matrix elements of the operator $\tilde{B}_{\text{c.m.}}^{(01)}$, rather than the matrix elements among individual κLJM substates, which are much greater in number.

To explicitly relate the null space problem at the level of individual states to that for SU(3) $\times$ SU(2)-reduced matrix elements, let us return for a moment to κLJM states and observe that any CMF state $|\Psi_{N_{\text{ex}}}^{\text{CMF}}[(\lambda\mu)S_pS_nS;\kappa LJM]\rangle$ within the $W_{N_{\text{ex}}}[(\lambda\mu)S_pS_nS]$ subspace must satisfy

$$\langle\Psi_{N_{\text{ex}}-1}[(\lambda'\mu')S_p'S_n'S';\kappa'L'J'M']|\tilde{B}_{\text{c.m.},L_0=1,M_0}^{(01)}|\Psi_{N_{\text{ex}}}^{\text{CMF}}[(\lambda\mu)S_pS_nS;\kappa LJM]\rangle = 0, \tag{6}$$

5

for every state $|\Psi_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S'_pS'_nS';\kappa'L'J'M']\rangle \in W_{N_{\mathrm{ex}}-1}$. Since we are working with states of good angular momentum, we can immediately rewrite the condition in terms of a reduced matrix element as

$$\langle\Psi_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S'_pS'_nS';\kappa'L'J']\|\tilde{B}^{(01)}_{\mathrm{c.m.},L_0=1}\|\Psi^{\mathrm{CMF}}_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS;\kappa LJ]\rangle = 0. \qquad (7)$$

Note that, since $\tilde{B}^{(01)}_{\mathrm{c.m.}}$ acts only on spatial degrees of freedom, we actually need only consider the case $(S'_pS'_nS') = (S_pS_nS)$. The ordinary SU(2)-reduced matrix element in (7) is related to the SU(3) × SU(2)-reduced matrix element of $\tilde{B}^{(01)}_{\mathrm{c.m.}}$ by the SU(3) Wigner-Eckart theorem (and LS-coupling relations), as

$$\langle\Psi_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S_pS_nS;\kappa'L'J']\|\tilde{B}^{(01)}_{\mathrm{c.m.},L_0=1}\|\Psi^{\mathrm{CMF}}_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS;\kappa LJ]\rangle$$
$$= (-)^{J+L'+1+S}\hat{L}'\hat{J}'\begin{Bmatrix} L & J & S \\ J' & L' & 1 \end{Bmatrix}\begin{pmatrix} (\lambda\mu) & (01) & \big\| & (\lambda'\mu') \\ \kappa L & 1 & & \kappa'L' \end{pmatrix}$$
$$\times \langle\Psi_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S_pS_nS]\|\tilde{B}^{(01)}_{\mathrm{c.m.}}\|\Psi^{\mathrm{CMF}}_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]\rangle, \quad (8)$$

where $\hat{J} \equiv (2J+1)^{1/2}$, and the quantity in parentheses is an SU(3) Clebsch-Gordan coefficient [29]. The condition that the complete set of SU(2)-reduced matrix elements appearing on the left-hand side of (8) vanish is equivalent to the condition that the single SU(3) × SU(2)-reduced matrix element on the right-hand side vanish.

Thus, for the CMF states, we seek SU(3)×SU(2)-reduced states $\|\Psi^{\mathrm{CMF}}_{N_{\mathrm{ex}}}[(\lambda\mu);S_pS_nS]\rangle$ such that

$$\langle\Psi_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S_pS_nS]\|\tilde{B}^{(01)}_{\mathrm{c.m.}}\|\Psi^{\mathrm{CMF}}_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]\rangle = 0, \qquad (9)$$

for all possible reduced states $\|\Psi_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S_pS_nS]\rangle \in W_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S_pS_nS]$. The subspaces $W_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S_pS_nS]$ which may be linked with $W_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]$ through $\tilde{B}^{(01)}_{\mathrm{c.m.}}$ are restricted by the SU(3) tensor character of $\tilde{B}^{(01)}_{\mathrm{c.m.}}$. Specifically, $(\lambda'\mu')$ must be contained in the product $(\lambda\mu) \times (01)$ which, from the general rules of SU(3) coupling [30], may be seen to consist of

$$(\lambda\mu) \times (01) = \begin{cases} (01) & \lambda = \mu = 0 \\ (0\ \mu+1) \oplus (1\ \mu-1) & \lambda = 0, \mu \geq 1 \\ (\lambda 1) \oplus (\lambda-1\ 0) & \lambda \geq 1, \mu = 0 \\ (\lambda\ \mu+1) \oplus (\lambda+1\ \mu-1) \oplus (\lambda-1\ \mu) & \lambda \geq 1, \mu \geq 1. \end{cases} \qquad (10)$$

The problem of finding reduced states which satisfy (9) can be converted into searching for the null space of a matrix, the entries of which are the SU(3) × SU(2)-reduced matrix elements of $\tilde{B}^{(01)}_{\mathrm{c.m.}}$ between the SU(3)×SU(2)-reduced basis states for the $W_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]$ subspace and the SU(3) × SU(2)-reduced basis states for each of the possible subspaces $W_{N_{\mathrm{ex}}-1}[(\lambda'\mu')S_pS_nS]$. The resulting matrix has the form illustrated in Fig. 1, where the horizontal dashed lines delimit submatrices corresponding to the different final spaces with $(\lambda'\mu') = (\lambda'_1\mu'_1), (\lambda'_2\mu'_2), \ldots$, as allowed by the selection rule (10). (There will be at most three such submatrices.) The entries of the null vectors then give the expansion coefficients for the basis states for the CMF space $W^{\mathrm{CMF}}_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]$ in terms of the original basis states of $W_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]$.

The SU(3)-reduced matrix elements of $\tilde{B}^{(01)}_{\mathrm{c.m.}}$ entering into the matrix of Fig. 1 can be calculated numerically using methods from Ref. [31]. In particular, the SU(3) × SU(2)

6

$$
\begin{bmatrix}
\langle\Psi^{(\lambda_1'\mu_1')}_{N_{\text{ex}}-1,1}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},1}\rangle & \langle\Psi^{(\lambda_1'\mu_1')}_{N_{\text{ex}}-1,1}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},2}\rangle & \cdots \\[4pt]
\langle\Psi^{(\lambda_1'\mu_1')}_{N_{\text{ex}}-1,2}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},1}\rangle & \langle\Psi^{(\lambda_1'\mu_1')}_{N_{\text{ex}}-1,2}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},2}\rangle & \cdots \\[4pt]
\vdots & \vdots & \\[4pt]
\hdashline
\langle\Psi^{(\lambda_2'\mu_2')}_{N_{\text{ex}}-1,1}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},1}\rangle & \langle\Psi^{(\lambda_2'\mu_2')}_{N_{\text{ex}}-1,1}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},2}\rangle & \cdots \\[4pt]
\langle\Psi^{(\lambda_2'\mu_2')}_{N_{\text{ex}}-1,2}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},1}\rangle & \langle\Psi^{(\lambda_2'\mu_2')}_{N_{\text{ex}}-1,2}\|\tilde{B}^{(01)}_{\text{c.m.}}\|\Psi^{(\lambda\mu)}_{N_{\text{ex}},2}\rangle & \cdots \\[4pt]
\vdots & \vdots & \\[4pt]
\hdashline
\vdots & \vdots &
\end{bmatrix}
$$

Figure 1: Form of the matrix representation of $\tilde{B}^{(01)}_{\text{c.m.}}$, as reduced matrix elements between the SU(3)-NCSM basis states for the $W_{N_{\text{ex}}}[(\lambda\mu)S_pS_nS]$ subspace (identified with the columns) and the SU(3)-NCSM basis states for each of the possible subspaces $W_{N_{\text{ex}}-1}[(\lambda'\mu')S_pS_nS]$ (identified with the rows).

matrix elements of a one-body operator such as $\tilde{B}^{(01)}_{\text{c.m.}}$ (or an n-body operator in general) can readily be computed, once the operator is expressed in second-quantized form in terms of SU(3) $\times$ SU(2)-coupled products of creation operators $a^{\dagger}_{(\eta0)1/2}$ and annihilation operators $\tilde{a}_{(0n)1/2}$ [27]. For the center-of-mass annihilation operator $\tilde{B}^{(01)}_{\text{c.m.}}$, the second-quantized form is obtained as

$$
\tilde{B}^{(01)}_{\text{c.m.}} = \frac{1}{\sqrt{A}}\sum_{\eta}\sqrt{\frac{(\eta+1)(\eta+2)}{3}}\langle\eta\|\tilde{b}^{(01)}\|\eta+1\rangle\left[a^{\dagger}_{(\eta0)1/2}\times\tilde{a}_{(0,\eta+1)1/2}\right]^{(01)0}, \quad (11)
$$

where $\langle\eta\|\tilde{b}^{(01)}\|\eta+1\rangle = \sqrt{\eta+3}$.

4. Dimensions of CMF spaces

Let us now examine the dimensions of the CMF subspaces obtained by the methods of Section 3. Our primary interest is in the distribution of CMF and spurious states with respect to the SU(3) $\times$ SU(2) quantum numbers. The Sp-NCSM approach requires identification of these CMF SU(3) $\times$ SU(2) irreps, at low N_{ex}, from which Sp(3, $\mathbb{R}$) irreps extending to high N_{ex} are created by repeated action of the symplectic raising operator (Section 1).

To begin with, the simplest illustration we might consider is the model space for the deuteron (^{2}H), which is shown along with that for the triton (^{3}H) in Fig. 2. The full SU(3)-NCSM space for the deuteron may be broken into subspaces $W_{N_{\text{ex}}}[(\lambda\mu)\frac{1}{2}\frac{1}{2}S]$, with $S = 0$ and 1. The dimensions of these subspaces — by which we specifically mean the number of SU(3) $\times$ SU(2)-reduced basis states, not the total number of κLJ basis states, which would be much higher — are indicated by the areas of the outer, light circles in Fig. 2. Then, for each value of N_{ex}, it is found that solution of the null space problem for the center-of-mass annihilation operator yields two CMF reduced states. Both have $(\lambda\mu) = (N_{\text{ex}}0)$, one with $S = 0$ and one with $S = 1$. These CMF subspaces are indicated by the inner, dark circles in Fig. 2.
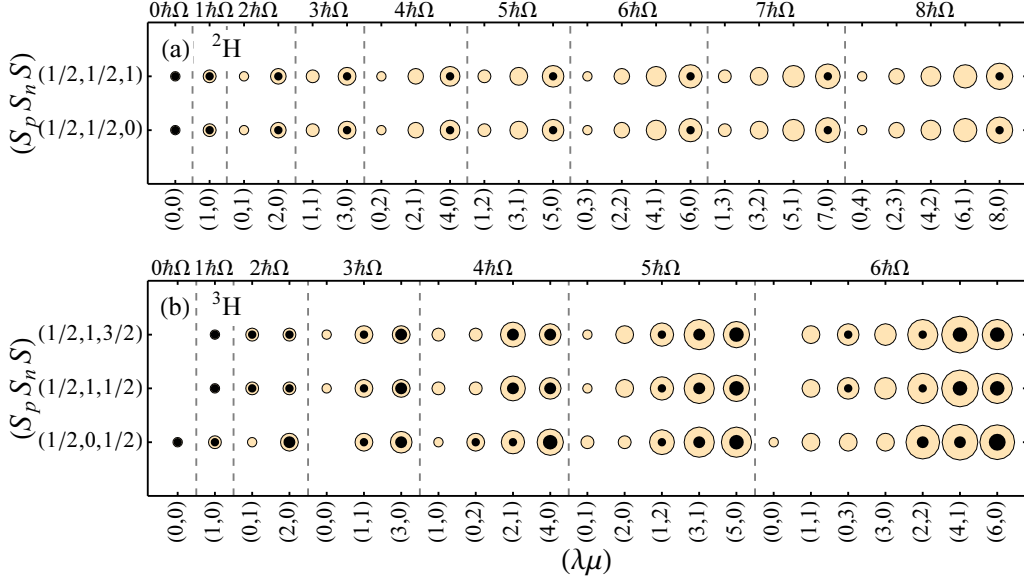
Figure 2: Dimensions of the SU(3) × SU(2)-reduced subspaces of the SU(3)-NCSM model space for (a) the deuteron (^{2}H) and (b) the triton (^{3}H). The area of the light (outer) circle indicates the full dimension, *i.e.*, of $W_{N_{ex}}[(\lambda\mu)S_pS_nS]$, and the area of the dark (inner) circle indicates the dimension of its CMF subspace, *i.e.*, of $W_{N_{ex}}^{CMF}[(\lambda\mu)S_pS_nS]$. Subspaces are arranged by N_{ex} (labeled by $N_{ex}\hbar\Omega$ at top), SU(3) quantum numbers (at bottom), and spin quantum numbers $(S_pS_nS) = (\frac{1}{2}\frac{1}{2}S)$ (at left).

The deuteron provides a particularly illuminating example, since the quantum numbers of the CMF spaces obtained in Fig. 2 may be understood through simple arguments. Let $N_{c.m.}$ and N_{rel} denote the number of oscillator excitations of the center-of-mass and relative degrees of freedom, respectively, so $N_{ex} = N_{c.m.} + N_{rel}$. The CMF condition imposes $N_{c.m.} = 0$ and thus $N_{rel} = N_{ex}$. For the two-particle system, the transformation between single-particle and relative coordinates is straightforward. There is only a single relative coordinate vector, and the harmonic oscillator in this coordinate is equivalent to the harmonic oscillator for a single particle in three dimensions. For a given N_{ex}, it will therefore carry SU(3) quantum numbers $(N_{ex}0)$. The center-of-mass oscillator carries (00) for a CMF state. Therefore the CMF state as a whole will have $(\lambda\mu) = (N_{ex}0) \times (00) = (N_{ex}0)$, as well. Since the deuteron consists of distinguishable particles, the coupling of spins is independent of the spatial degrees of freedom, and both $S = 0$ and 1 are obtained.

In general, as we move beyond the two-body problem, the fraction of the model space dimension which corresponds to CMF states, versus that which corresponds to spurious states, depends both on the number of nucleons and on the number N_{ex} of oscillator quanta. The spurious contribution at $N_{ex} = 0$ is identically vanishing, as shown by Elliott and Skyrme [15]. For a given nucleus, the spurious contribution becomes an increasing fraction of the total space with increasing N_{ex}, while, for a given level of excitation N_{ex}, the spurious contribution becomes a less significant fraction of the total space with increasing atomic mass A. These trends are already in evidence in comparing deuterium with tritium (Fig. 2) but may be seen more systematically in Fig. 3(a), where
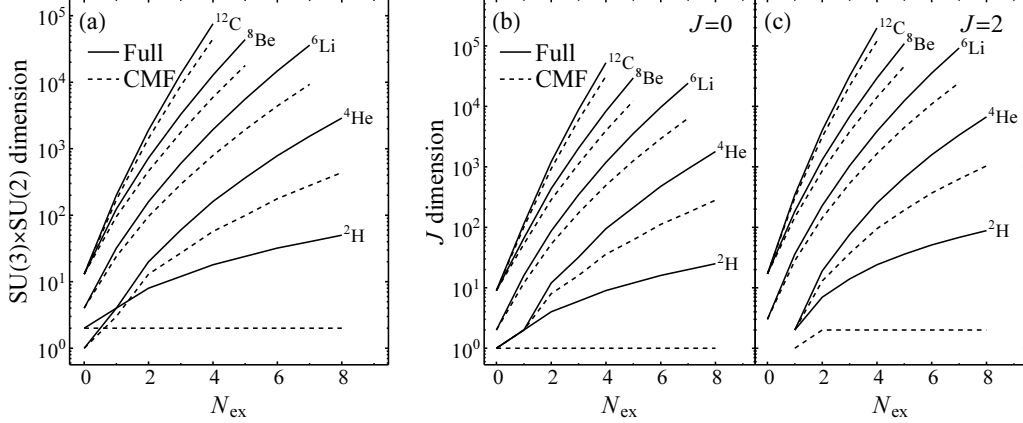
Figure 3: Dimension of the SU(3)-NCSM model space, decomposed according to N_{ex}: (a) by number of SU(3) × SU(2)-reduced basis states, (b) after branching to $J = 0$ states, and (c) after branching to $J = 2$ states. Both full (solid curves) and CMF (dashed curves) dimensions are shown, for ^{2}H, ^{4}He, ^{6}Li, ^{8}Be, and ^{12}C.

the dimensions of the full spaces (solid curves) and CMF spaces (dashed curves) are shown, as functions of N_{ex}, for several nuclei with $2 \leq A \leq 12$.

Qualitatively, the pattern in the evolution of the CMF fraction may be understood from simple counting arguments, by considering the possible ways of distributing N_{ex} oscillator quanta over the $3A$ oscillator degrees of freedom of the nuclear system. These may be decomposed into three center-of-mass oscillator degrees of freedom and $3A - 3$ relative oscillator degrees of freedom. If many oscillator quanta are to be distributed over few degrees of freedom ($N_{ex} \gg A$), most of the distributions will allocate at least one oscillator quantum to the center-of-mass degrees of freedom, leading to a high proportion of spurious states, $i.e.$, a smaller CMF fraction. Conversely, if few oscillator quanta are to be distributed over many degrees of freedom ($N_{ex} \ll A$), most distributions will "miss" these three center-of-mass degrees of freedom, $i.e.$, not allocate any oscillator quanta to them, leading to a low proportion of spurious states, $i.e.$, a larger CMF fraction.[2]

We focus now on the detailed distribution of CMF and spurious states over the SU(3) × SU(2) subspaces of $W_{N_{ex}}$, that is, the $N_{ex}(\lambda\mu)S_p S_n S$ subspaces of Section 3. First, it should be noted that the dimensions of these subspaces vary widely. The dimensions of the SU(3)×SU(2) subspaces for $^4_2$He$_2$, $^6_3$Li$_3$, and $^8_4$Be$_4$, with $N_{ex} \leq 8$, 6, and 4, respectively, are shown in Fig. 4 — these dimensions vary from one to 640. To accommodate this range, the circles in Fig. 4 have been sized according to a power law scale, such that a doubling in radius represents a tenfold increase in dimension. However, any such nonlinear rescaling precludes meaningful visual comparison of the dimensions of the full and CMF subspaces, as was possible in Fig. 2. Consequently, we examine the CMF

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[2]Quantitatively, such counting arguments give an estimated CMF fraction $(\dim W^{CMF}_{N_{ex}})/(\dim W_{N_{ex}}) \approx (3A - 1)^{\underline{3}}/(N_{ex} + 3A - 1)^{\underline{3}}$, where $m^{\underline{n}} \equiv m(m - 1) \cdots (m - n + 1)$. This expression gives the exact result for the deuteron, when applied to the total space, $i.e.$, counting all M substates, but is of only approximate validity for other nuclei, due to neglect of antisymmetrization. For large N_{ex}, we obtain a CMF fraction falling as N_{ex}^{-3}.
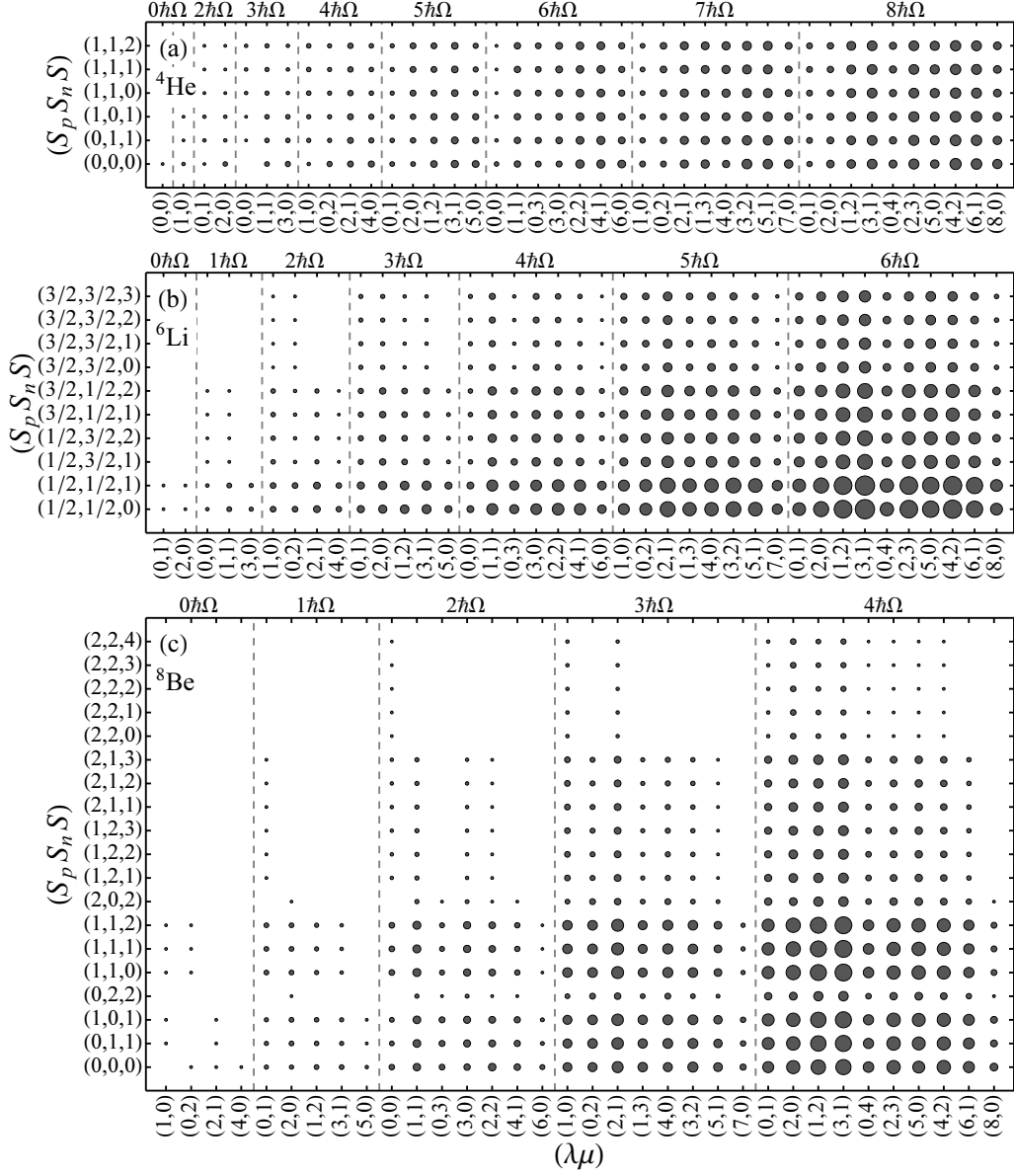
Figure 4: Dimensions of the SU(3) × SU(2)-reduced subspaces for (a) ^{4}He, (b) ^{6}Li, and (c) ^{8}Be. The size of each circle represents the dimension, scaled such that a doubling in radius represents a tenfold increase in dimension. Subspaces are arranged by $N_{\mathrm{ex}}(\lambda\mu)S_p S_n S$ as indicated in the caption to Fig. 2.
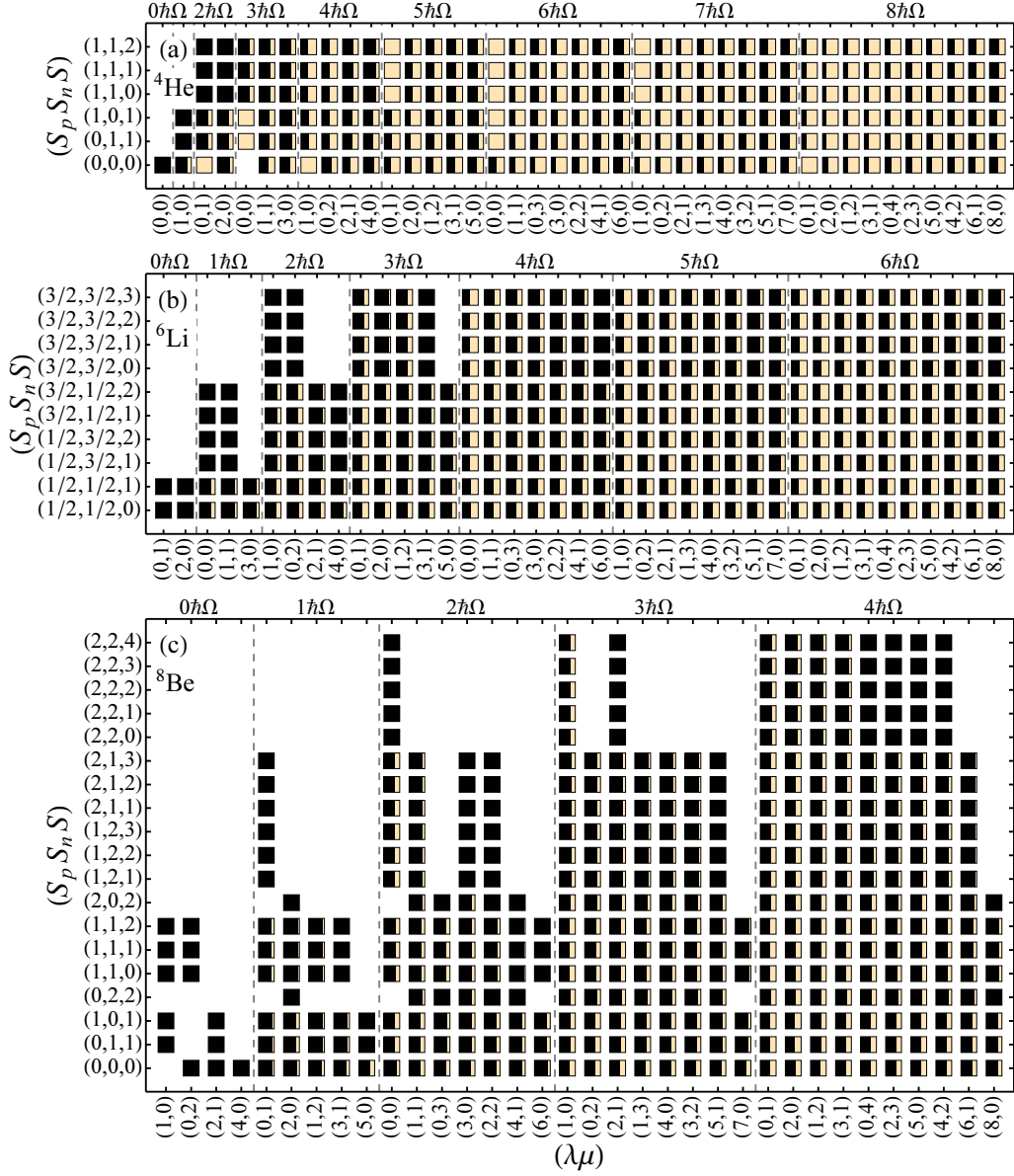
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Figure 5: Ratio of CMF dimension to total dimension, for the SU(3) × SU(2)-reduced subspaces for (a) ^{4}He, (b) ^{6}Li, and (c) ^{8}Be. The area of the darkened portion of each square, relative to the total area, indicates the dimension of the CMF subspace, *i.e.*, of $W_{N_{\mathrm{ex}}}^{\mathrm{CMF}}[(\lambda\mu)S_pS_nS]$ relative to that of the full subspace, *i.e.*, of $W_{N_{\mathrm{ex}}}[(\lambda\mu)S_pS_nS]$. Subspaces are arranged by $N_{\mathrm{ex}}(\lambda\mu)S_pS_nS$ as indicated in the caption to Fig. 2.

fractions, *i.e.*, the ratio $(\dim W_{N_{\mathrm{ex}}}^{\mathrm{CMF}}[(\lambda\mu)S_p S_n S])/(\dim W_{N_{\mathrm{ex}}}[(\lambda\mu)S_p S_n S])$, separately in Fig. 5, for these same nuclei.

As already noted, the CMF fractions decrease with increasing N_{ex} and approach unity, for a given N_{ex}, with increasing mass. However, within each N_{ex} space, demarcated by vertical dashed lines in Fig. 5, a further dominant trend may be noticed in the variation of CMF fractions among the SU(3)×SU(2) subspaces. It is observed that the spurious states are preferentially found in the subspaces with SU(3) quantum numbers corresponding to the lowest values of the SU(3) second-order Casimir invariant C_2, while the CMF states are preferentially found in the subspaces corresponding to the highest eigenvalues of C_2. In Fig. 5 (as well as in Figs. 2 and 4), within each $W_{N_{\mathrm{ex}}}$, the SU(3) irrep labels $(\lambda\mu)$ are ordered from left to right by increasing eigenvalue of C_2 (given by $\langle C_2 \rangle = \lambda^2 + \lambda\mu + \mu^2 + 3\lambda + 3\mu$), where labels which are degenerate with respect to C_2 are then ordered by increasing λ. The lowest CMF fractions are (predominantly) found at left, and the highest (predominantly) at right. While some evidence may be seen for patterns in the distribution with respect to the spin labels, these are not as clear or consistent.

So far, we have considered dimensions at the level of SU(3) × SU(2)-reduced basis states. We may also deduce from these the full and CMF dimensions in terms of J-coupled states. Although much of the computational process in an SU(3)-NCSM calculation can be carried out in terms of SU(3) × SU(2)-reduced states, and it is these reduced states which are relevant to the definition of the Sp-NCSM model space, the Hamiltonian matrix in an SU(3)-NCSM calculation must ultimately be realized in terms of basis states of definite angular momentum J. As outlined in Section 2, the J states are obtained by first branching each SU(3) × SU(2)-reduced state (1) to states of definite orbital angular momentum L. The L values contained within an SU(3) irrep $(\lambda\mu)$ are given by the SU(3) → SO(3) branching rule [4].[3] Then L is coupled with S to yield states of total angular momentum J according to the usual coupling rules for angular momentum addition. The dimensions of the resulting J-spaces — both the full space and its CMF portion — are shown for several light nuclei in Fig. 3(b,c), for $J = 0$ and $J = 2$, respectively. Although the dimensions of the J-spaces are calculated here via the SU(3) × SU(2) coupling scheme, the results obtained are generally applicable to any J-coupled scheme for the NCSM, in an N_{max} truncation.

5. Conclusions

The separation or elimination of spurious center-of-mass excitations is essential to the problem of determining the intrinsic structure of nuclei. If an SU(3)-coupled harmonic oscillator basis is used for the many-body problem, as in the SU(3)-NCSM, the separation may be carried out at the level of SU(3) irreps, in particular, within subspaces of fixed number of oscillator quanta and $(\lambda\mu)S_p S_n S$ labels. We have formulated the problem of finding the CMF subspace as a matrix null-space problem, based on the SU(3) × SU(2)-reduced matrix elements of the center-of-mass annihilation operator, which is solved independently for each SU(3)×SU(2) subspace of the full model space. It

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[3]For each value $K = \min(\lambda, \mu) \bmod 2, \ldots, \min(\lambda, \mu) - 2, \min(\lambda, \mu)$, states are obtained with $L = K, K+1, \ldots, K+\max(\lambda, \mu)$, with the exception that $L = \max(\lambda, \mu) \bmod 2, \ldots, \max(\lambda, \mu) - 2, \max(\lambda, \mu)$ if $K = 0$.

is therefore possible to remove spurious contributions from the SU(3)-NCSM model space *prior* to diagonalization of the Hamiltonian, rather than through a Lawson term. In the context of the SU(3)-NCSM *per se*, this raises the possibility of substantial reductions in dimensionality of the problem, principally in the high N_{ex} subspaces of lighter nuclei.

However, a more essential application lies in providing the foundation for ensuring exact separation of center-of-mass and intrinsic dynamics, or removal of spurious contributions, in the Sp-NCSM. The purpose of the Sp-NCSM is to incorporate physically relevant portions of the model space extending to much higher numbers of oscillator quanta, beyond those which can be practically reached if one must retain the complete $N_{ex}(\lambda\mu)S_p S_n S$ subspaces of the SU(3)-NCSM. However, factorization of center-of-mass and intrinsic wave functions is still guaranteed if the $Sp(3, \mathbb{R})$ basis is constructed starting from SU(3)-NCSM extremal states which are free of spurious excitation. The present approach may also serve as the starting point for eliminating spurious admixtures in other extensions to the SU(3)-NCSM, such as an adaptation of the importance truncation scheme [32] to the SU(3)-NCSM.

Acknowledgements

References

[1] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. 84 (2000) 5728.
[2] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. C 62 (2000) 054311.
[3] P. Navrátil, S. Quaglioni, I. Stetcu, and B. R. Barrett, J. Phys. G 36 (2009) 083101.
[4] J. P. Elliott, Proc. R. Soc. London A 245 (1958) 128.
[5] J. P. Elliott, Proc. R. Soc. London A 245 (1958) 562.
[6] J. P. Elliott and M. Harvey, Proc. R. Soc. London A 272 (1963) 557.
[7] G. Rosensteel and D. J. Rowe, Phys. Rev. Lett. 38 (1977) 10.
[8] G. Rosensteel and D. J. Rowe, Ann. Phys. (N.Y.) 126 (1980) 343.
[9] J. P. Draayer, K. J. Weeks, and G. Rosensteel, Nucl. Phys. A 413 (1984) 215.
[10] T. Dytrych, K. D. Sviratcheva, C. Bahri, J. P. Draayer, and J. P. Vary, Phys. Rev. Lett. 98 (2007) 162503.
[11] T. Dytrych, K. D. Sviratcheva, C. Bahri, J. P. Draayer, and J. P. Vary, Phys. Rev. C 76 (2007) 014315.
[12] T. Dytrych, J. P. Draayer, K. D. Launey, M. A. Caprio, and D. Langr, J. Phys. Conf. Ser. (in press).
[13] T. Dytrych, K. D. Launey, P. Maris, M. A. Caprio, J. P. Draayer, J. P. Vary, and D. Langr (in preparation).
[14] T. Dytrych, K. D. Sviratcheva, J. P. Draayer, C. Bahri, and J. P. Vary, J. Phys. G 35 (2008) 123101.
[15] J. P. Elliott and T. H. R. Skyrme, Proc. R. Soc. London A 232 (1955) 561.
[16] E. Baranger and C. W. Lee, Nucl. Phys. 22 (1961) 157.
[17] H. J. Lipkin, Phys. Rev. 110 (1958) 1395.
[18] J. B. McGrory and B. H. Wildenthal, Phys. Lett. B 60 (1975) 5.
[19] M. A. Caprio, P. Maris, and J. P. Vary, Phys. Rev. C 86 (2012) 034312.
[20] D. H. Gloeckner and R. D. Lawson, Phys. Lett. B 53 (1974) 313.

[21] M. Kretzschmar, Z. Phys. 158 (1960) 284.

[22] B. J. Verhaar, Nucl. Phys. 21 (1960) 508.

[23] K. T. Hecht, Nucl. Phys. A 170 (1971) 34.

[24] D. J. Millener and D. Kurath, Nucl. Phys. A 255 (1975) 315.

[25] D. J. Millener, in *Group Theory and Special Symmetries in Nuclear Physics*, edited by J. P. Draayer and J. Jänecke (World Scientific, Singapore, 1992), p. 276.

[26] F. Q. Luo, M. A. Caprio, and T. Dytrych, J. Phys. Conf. Ser. (in press).

[27] J. Escher and J. P. Draayer, J. Math. Phys. 39 (1998) 5123.

[28] J. P. Draayer, Y. Leschber, S. C. Park, and R. Lopez, Comput. Phys. Commun. 56 (1989) 279.

[29] Y. Akiyama and J. P. Draayer, Comput. Phys. Commun. 5 (1973) 405.

[30] M. F. O'Reilly, J. Math. Phys. 23 (1982) 2022.

[31] C. Bahri and J. P. Draayer, Comput. Phys. Commun. 83 (1994) 60.

[32] R. Roth, Phys. Rev. C 79 (2009) 064324.